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ADP012103

TITLE: Chemical Kinetics and Aerodynamics of Ignition

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TITLE: Army Research Office and Air Force Office of Scientific Research. Contractors' Meeting in Chemical Propulsion [2001] Held in the University of Southern California on June 18-19, 2001

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# CHEMICAL KINETICS AND AERODYNAMICS OF IGNITION

(ARO Grant No. DAAG19-01-0004)

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## SUMMARY/OVERVIEW

This program investigates ignition of nonhomogenous systems, such as those found in practical combustion devices, by looking at ignition in a counterflow. During the reporting period, major effort was expanded on ignition in a nonpremixed turbulent counterflow where a hot air jet ignites an ambient temperature fuel jet. Specifically, the non-reacting turbulent flow was first investigated experimentally to provide data in support of other ignition and turbulence modeling studies. Subsequently, experiments were conducted to determine the ignition temperatures over a range of fuel concentrations, pressures, and strain rates. Preliminary modeling of turbulent ignition was also accomplished by first solving for the flow field using a Reynolds stress model and then solving for the chemistry by using a joint scalar PDF equation and Monte Carlo techniques. This two step approach is possible because of the small amount of heat release prior to ignition.

## TECHNICAL DISCUSSION

### 1. Characterization of non-reacting turbulent flow fields

High fidelity experimental data for turbulent non-reacting counterflows are necessary to interpret turbulent non-premixed ignition experiments and to develop and evaluate numerical models for turbulent ignition. It is particularly important to have measurements of counterflows where one jet has a significantly different density than the other, as such data is not available in the literature. Counterflowing jets of heated air and cold nitrogen were investigated using a two-component laser Doppler anemometry system to measure velocity moments, spectra, and autocorrelations throughout the flow field. Operating conditions spanned a range of pressures, bulk strain rates, perforated plate configurations, and air temperatures. In addition to measuring velocity moments along the counterflow axis, mean and fluctuating velocity profiles were made in the radial direction at each nozzle exit. These profiles are important for establishing boundary conditions in turbulent flow models. The radial velocity gradients are needed in quasi-one dimensional turbulence models and the profiles themselves are needed for higher dimensional Reynolds stress models and Large Eddy Simulations.

Autocorrelation measurements at the burner exits were used with Taylor's hypothesis to estimate the flow's integral length scale. The length scales were about 70% of the perforated plate hole diameters, in agreement with theory and other experiments. The length scale is important for modeling efforts since it can be used to estimate the turbulent dissipation rate.

Turbulent power spectra were determined at the burner exits to further characterize the turbulence for a given perforated plate configuration. For example, due to the difficulties associated with generating turbulence in a strongly heated flow, some experiments have been conducted with only one perforated plate, located in the cold flow. The use of this configuration

was justified by the observation that the turbulent fluctuations look like those in a turbulent counterflow that has perforated plates in both nozzles as shown in Fig. 1. However, a comparison of the power spectra measured at the hot side of the burner, Fig. 2, shows that there is a significant difference between the two cases. The spectrum of the case without a second perforated plate is suggestive of very young, undeveloped turbulence, indicating that it is important to have a perforated plate in both sides of the burner when studying turbulence.

## 2. Turbulent non-premixed ignition experiments

Earlier experiments on ignition in non-homogenous systems have either looked at laminar ignition or ignition in an atmospheric turbulent counterflow with only one perforated plate. Since most practical combustion systems are turbulent and, as noted above, two perforated plates are necessary to produce well-characterized turbulence, the earlier work has been extended. The non-premixed ignition temperature was measured in a turbulent counterflow generated by two perforated plates for a range of hydrogen concentrations, bulk strain rates, and pressures. The effect of fuel concentration is shown in Fig. 3. The increasing sensitivity as the fuel concentration decreases and the nearly constant ignition temperature at higher fuel concentrations are qualitatively similar to what was observed in previous non-premixed ignition studies for both hydrogen and other fuels. For all the cases shown, ignition was repeatable and once ignited the turbulent flame persisted, even when the air temperature was subsequently reduced. For lower concentrations, intermittent ignition was observed where above a certain temperature a flame would be repeatedly ignited and extinguished. No hysteresis was observed.

The effect of pressure on ignition is shown in Fig. 4. In light of the laminar hydrogen ignition results, the turbulent data are indicative of a transition between the dominance of second limit chemistry at lower pressures to third limit behavior at the highest pressures. This data will be crucial to evaluating turbulent ignition models because hydrogen displays a significantly higher sensitivity to changes in pressure than changes in other parameters.

## 3. Modeling of turbulent non-premixed ignition

The complex non-linear interactions between reaction, convection, diffusion, and turbulence make general modeling of turbulent reacting flows very difficult. Modeling turbulent ignition, however, is somewhat simplified by the fact that prior to ignition there is very little heat release and consequently, the chemistry does not significantly alter the velocity field. To take advantage of this situation, turbulent ignition modeling is being addressed in two steps. In the first step, the non-reacting flow field is solved using a Reynolds stress turbulence model and assuming pure mixing. These calculations have been found to be in reasonable agreement with experimental measurements. Chemistry is treated in the second step by using Monte Carlo methods to solve a joint scalar PDF transport equation for the previously calculated flow conditions. With this approach, a detailed hydrogen-oxygen mechanism can be used. Preliminary calculations show that an ignition kernel can be identified through the mean radical concentrations. It is also found that the peak concentrations increase gradually as the air temperature increases until there is a sudden acceleration as ignition occurs.

## 4. Augmented Reduced Mechanism for Methane Oxidation with NO<sub>x</sub> Chemistry

We have previously proposed the concept of developing Augmented Reduced Mechanisms (ARM) for the description of chemical kinetics in complex situations. The primary premise is that while simplifications of detailed reaction mechanisms must be made for the description of chemistry in complex flows, they have to remain sufficiently comprehensive in terms of the system dependence on temperature, pressure and concentration in order to retain the essential

chemical information. As such, existing reduced mechanisms that typically consist of four to five steps have been shown that, while simple and physically illuminating, they have restricted ranges of comprehensiveness. Consequently, a 12-step, sixteen species augmented reduced mechanism has been developed for methane oxidation that has shown a high degree of comprehensiveness in its ability to simulate the global responses of various combustion phenomena over extensive ranges of system parametric variations. The validation has now been extended to the temporal and spatial profiles of the temperature and species (both major and minor) concentrations.

The 12-step mechanism for methane oxidation has been extended to account for NO formation, with a 14-step mechanism to describe the thermal, prompt, and nitrous oxide mechanism, and a 15-step mechanism to include the NH<sub>3</sub>-related reactions. These ARMs demonstrate good performance in simulating results from the detailed mechanism.

#### MAJOR PUBLICATIONS

- [1] "Ignition of CO/H<sub>2</sub>/N<sub>2</sub> versus Heated Air in Counterflow: Experimental and Modeling Results," by C.G. Fotache, Y. Tan, C.J. Sung and C.K. Law, *Combustion and Flame*, Vol. 120, pp. 417-426 (2000).
- [2] "Non-Premixed Ignition of n-Heptane and iso-Octane in a Laminar Counterflow," by J.D. Blouch and C.K. Law, *Proceedings of the Combustion Institute*, Vol. 28, pp. 1679-1686 (2000).
- [3] "Further Validation of an Augmented Reduced Mechanism for Methane Oxidation: Comparison of Global Parameters and Detailed Structure," by C.J. Sung, C.K. Law, and J.Y. Chen, *Combustion Science and Technology*, Vol. 150, pp. 201-220 (2000).
- [4] "Augmented Reduced Mechanisms for NO Emission in Methane Oxidation," by C. J. Sung, C.K. Law, and J.Y. Chen, *Combustion and Flame*, in press.

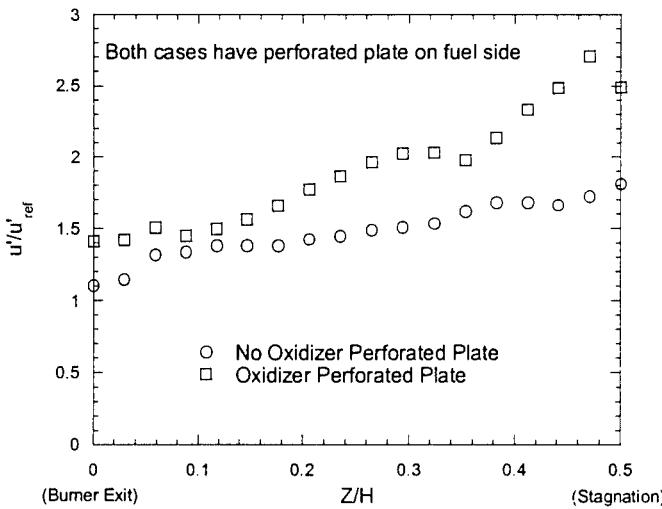


Figure 1: Velocity fluctuations on oxidizer side of stagnation plane.

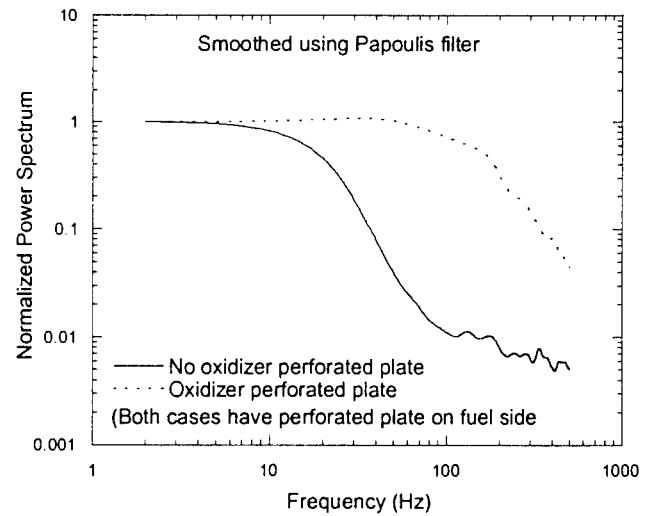


Figure 2: Power spectrum at oxidizer exit ( $Z=0$ ) normalized by value at 2Hz.

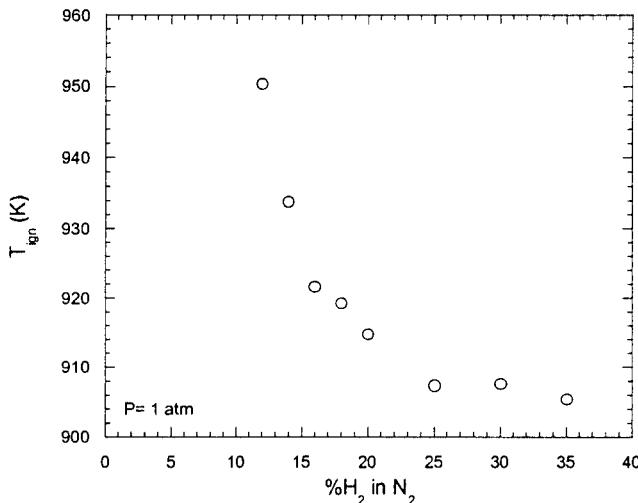


Figure 3: Effect of fuel concentration on ignition temperature.

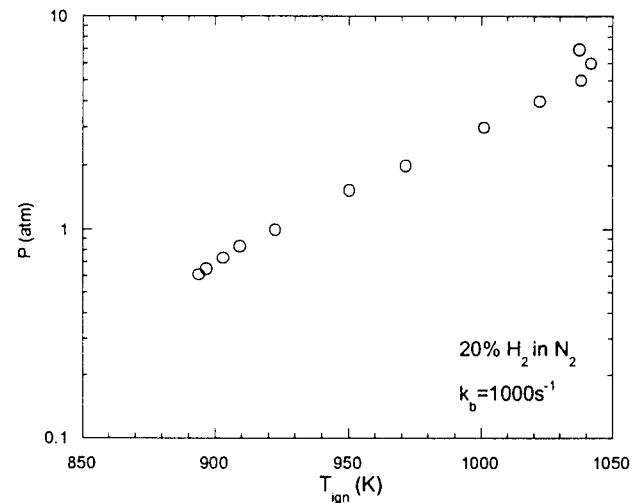


Figure 4: Effect of pressure on ignition temperature.